SOV/124-57-5-5858

Translation from: Referativnyy zhurnal. Mekhanika, 1957, Nr 5, p 119 (USSR)

AUTHOR: Sokolov, N. B.

TITLE: Concerning the Stress-strain Equations Depicting Large Planar Deformations (Ob uravneniyakh svyazi mezhdu napryazheniyami i bol'shimi deformatsiyami pri ploskom deformirovannom sostoyanii)

PERIODICAL: Tr. Penzensk. industr. in-ta, 1955, Nr 3, pp 14-23

ABSTRACT: The author examines the phenomenon of planar deformation. The components of a finite deformation are expressed in terms of the displacement functions. He determines the principal elongations and the directions of the principal axes both before and after deformation. By introducing certain auxiliary quantities he is enabled to evolve an equation wherein the stress components are expressed explicitly in terms of the generalized strain components. From the expressions obtained it is possible to evolve both the Hooke equations for small elastic deformations and the Hencky equations for small elastic-plastic deformations. The stress-strain ratio can be obtained by replacing the usual strain-component term with a term adjusted for the ratio of the postdeformation surface-area increment to the

Card 1/2

Concerning the Stress-strain Equations Depicting Large Planar Deformations

initial predeformation surface area. It is found that the tangential (shear) stress is a function of the triaxial deformation.

V. G. Osipov

AUTHOR: Sokolov, N.B., Doctor of Technical Sciences.

TITLE: Analysis of the operation of shaft mills and generalisation of experimental data. (Analiz raboty shakhtnykh melnits i obobshenie opytnykh dannykh.)

PERIODICAL: "Energomashinostroenie," (Power Machinery Construction), 1957, No. 3, pp. 7 - 12, (U.S.S.R.)

ABSTRACT: Evaluation and generalisation of the validity of test results obtained on industrial shaft mills during tests in crushing of coal, shale and milling peat, carried out by various authors during the last 15 to 20 years. The general preliminary analysis of the experimental data reveals the following basic features of mill operation: on feeding the fuel into the mill, operating under no-load conditions, the grinding takes place practically without any change in the required power, up to a certain limit in the quantity of the fed-in fuel. Further increase of the feeding-in of the fuel will bring about an increase in the required power, simultaneously with an increase of output; this increase in power continues up to a certain limit after which the operation of the mill becomes unstable and impossible owing to flooding of the mill by fuel. During the steady state operation of the mill, disregarding recirculation, the quantity of fed-in raw coal is equal to the quantity of pulverised coal produced by the mill. The calculation formula is based on empirical

Analysis of the operation of shaft mills and generalisation of experimental data. (Cont.)

values of the experimental data, given in the graph, Fig. 5, which yields for the power consumption the formula expressed by eq. (9), p.9, and the author claims that calculations obtained by means of this formula are in good agreement with experimentally-determined values (2). The relations are also derived for the wear and service life of the crushing elements; the eq. (12), p.11, expresses the relation derived by the author for the service life. By means of this formula, nomograms can be calculated, which facilitate the selection of shaft mills for given conditions of operation and an example of such a selection has been given in an earlier paper by the author for axial mills (2). In the final part of the paper, formulae are derived for milling peat, eqs. (14) and (15), p.12, and it can be seen from eq. (15) that the specific power consumption during grinding of milling peat increases with increasing diameter and r.p.m. of the rotor, whilst, in the case of coal, the power consumption decreases with increasing r.p.m.

9 graphs, 2 tables. 6 Russian and 1 German reference.

SOKOLOV, N.B.

Relationship between the components of stress and the components of finite plain strain. Uch. zap. PPI no.1:17-26 '63. (MIRA 17:2)

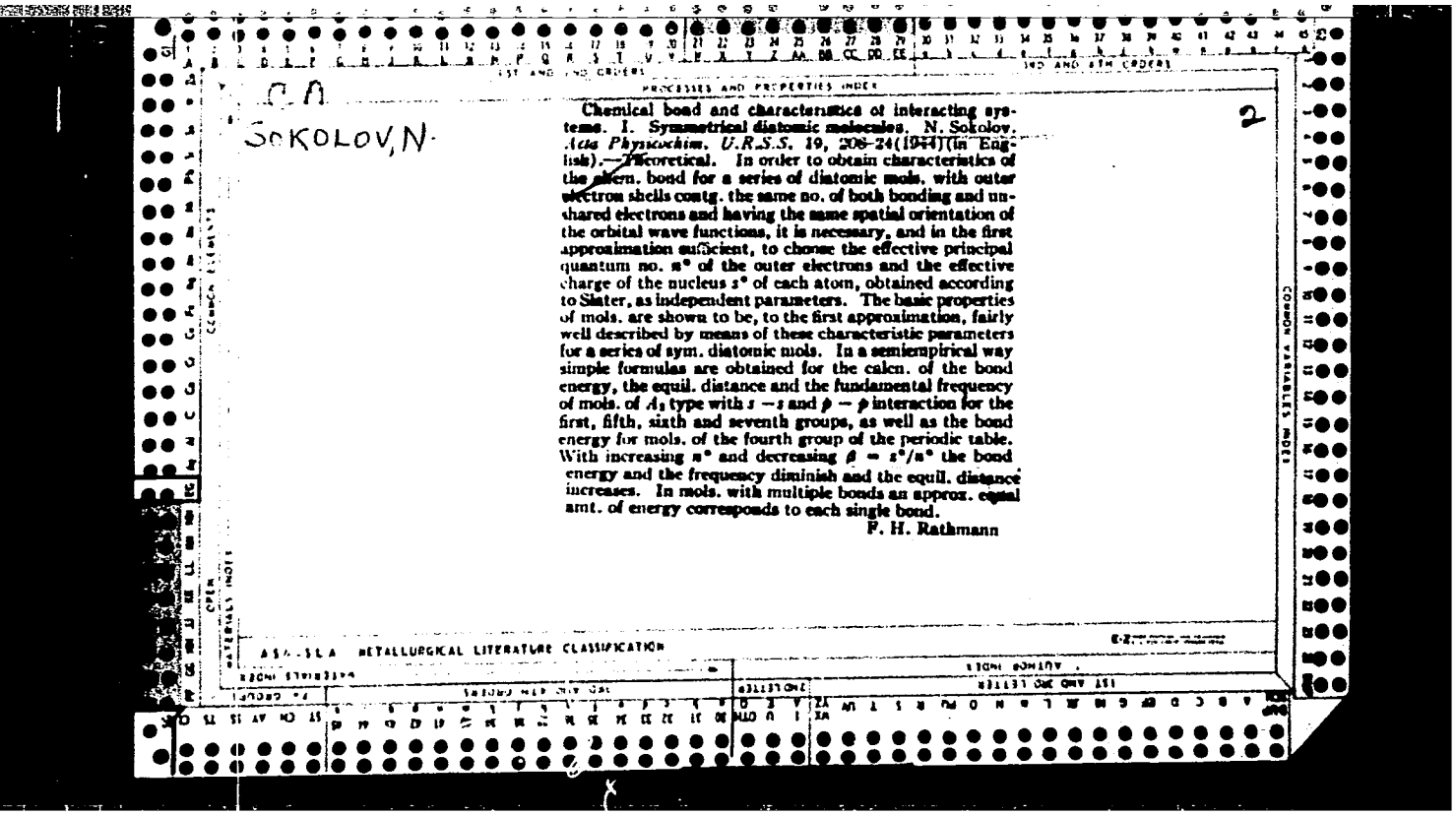
PSHENICHNOV, Ye.A.; SOKOLOV, N.D.

Eigenvalues and the probabilities of quantum transitions in a double asymmetrical potential well. Opt. i spektr. 17 no.3:343-348 S '64. (MIRA 17:10)

KAZHIGA, V.V.; SOKOLOV, N.D.

Unidimensional model of interaction between a diatomic radical and a solid surface. Kin. i kat. 6 no. 6:961-967 N-D '65 (MIRA 19:1)

1. Institut khimicheskoy fiziki AN SSSR. Submitted September 9, 1964.



C.A.

SOKOLOV, N.

2

Chemical bond and characteristics of interacting systems. I. Symmetrical diatomic molecules. N. Sokolov. *Acta Physicochim. U.R.S.S.* 19, 208-24(1944)(in English).—Theoretical. In order to obtain characteristics of the chem. bond for a series of diatomic mols. with outer electron shells contg. the same no. of both bonding and unshared electrons and having the same spatial orientation of the orbital wave functions, it is necessary, and in the first approximation sufficient, to choose the effective principal quantum no. n^* of the outer electrons and the effective charge of the nucleus s^* of each atom, obtained according to Slater, as independent parameters. The basic properties of mols. are shown to be, to the first approximation, fairly well described by means of these characteristic parameters for a series of sym. diatomic mols. In a semiempirical way simple formulas are obtained for the calcn. of the bond energy, the equil. distance and the fundamental frequency of mols. of A_2 type with $s-s$ and $p-p$ interaction for the first, fifth, sixth and seventh groups, as well as the bond energy for mols. of the fourth group of the periodic table. With increasing n^* and decreasing $\beta = s^*/n^*$ the bond energy and the frequency diminish and the equil. distance increases. In mols. with multiple bonds an approx. equal amt. of energy corresponds to each single bond.

F. H. Rathmann

PA 18T83

SOKOLOV, N. D.

USSR/Chemistry - Bonds, Hydrogen
Chemistry - Reaction Rates

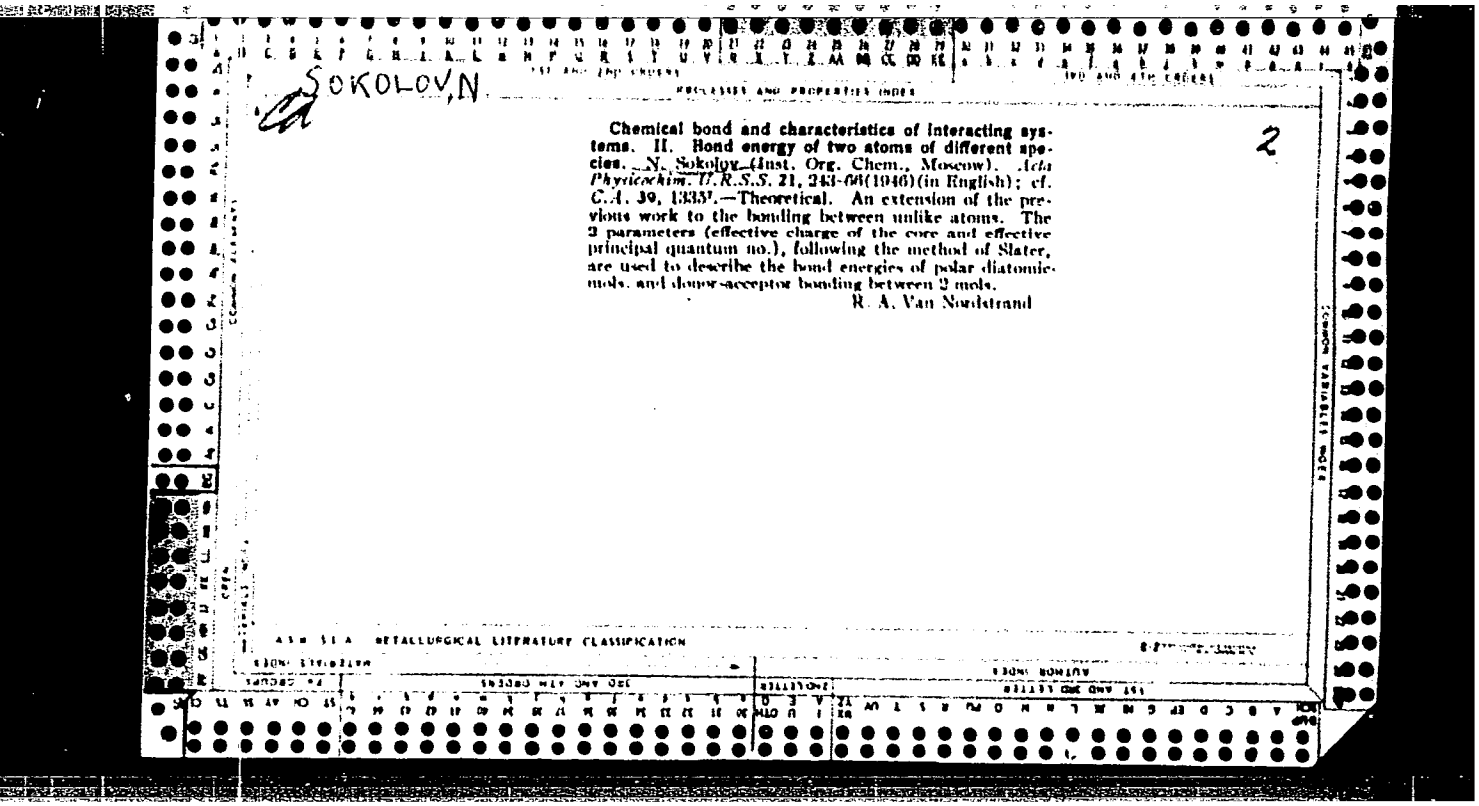
Jun 1946

"The Nature of the Hydrogen Bond, and the Effect of Complex Formation upon Reaction Rates," N. D. Sokolov, 2 pp

"Zhur Fiz Khim" Vol XX, No 6

Claim by the author that the reasoning shown in his article, spread over more sound cases, would be the path toward the solution of the problem of the influence of complex formations on reaction rates.

18T83



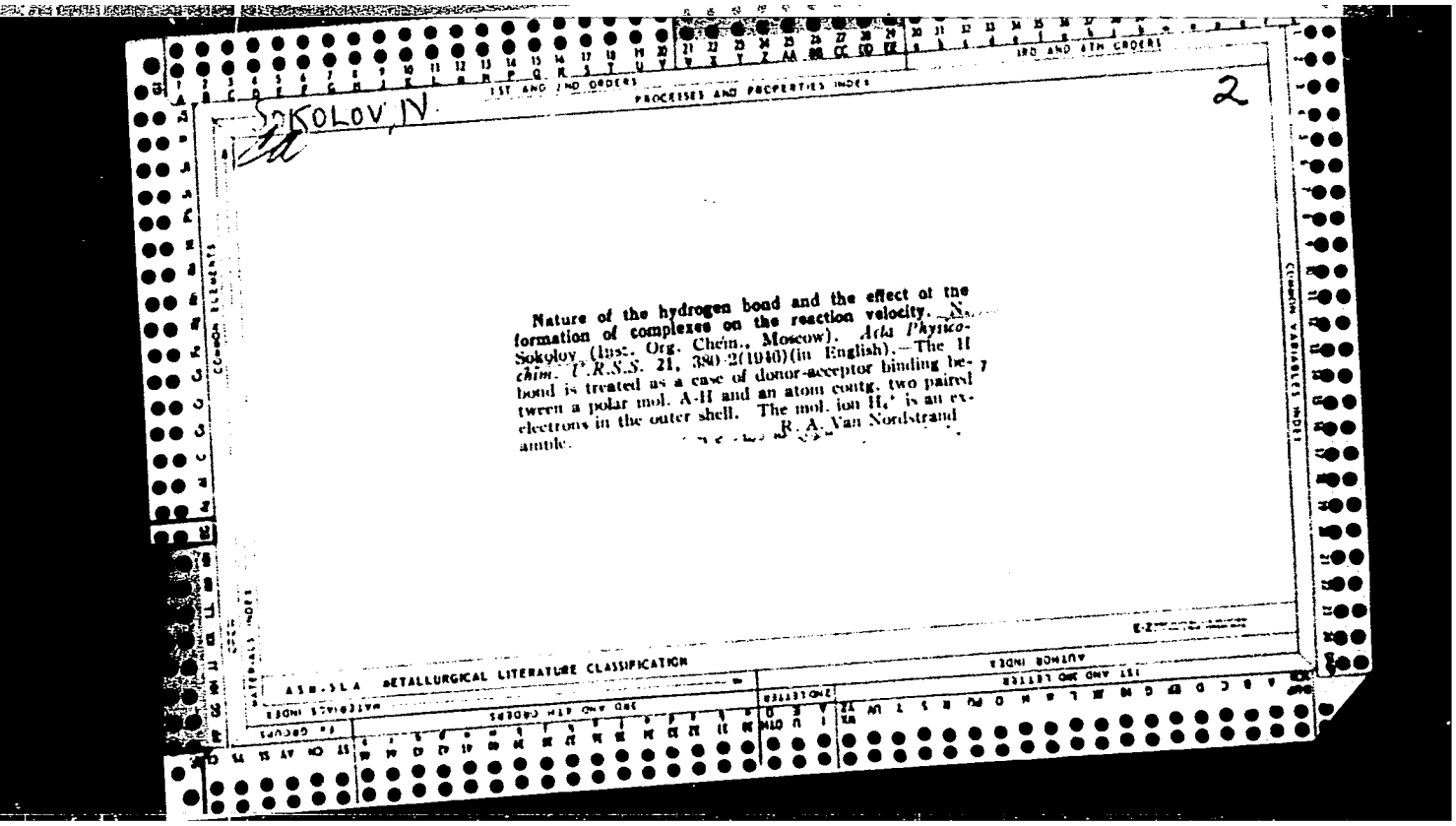
SOKOLOV, N.

Chemical bond and characteristics of interacting systems. II. Bond energy of two atoms of different species. N. Sokolov (Inst. Org. Chem., Moscow). *Acta Physicochim. U.R.S.S.* 21, 243-66(1946)(in English); cf. *C.A.* 39, 1333'.—Theoretical. An extension of the previous work to the bonding between unlike atoms. The 2 parameters (effective charge of the core and effective principal quantum no.), following the method of Slater, are used to describe the bond energies of polar diatomic mols. and donor-acceptor bonding between 2 mols.

R. A. Van Nordstrand

2

ASM SLA METALLURGICAL LITERATURE CLASSIFICATION



Nature of the hydrogen bond and the effect of the formation of complexes on the reaction velocity. N. Sokoloy (Inst. Org. Chem., Moscow). *Acta Physicochim. U.R.S.S.* 21, 380-2(1940)(in English).—The H bond is treated as a case of donor-acceptor binding between a polar mol. A-H and an atom contg. two paired electrons in the outer shell. The mol. ion H_3^+ is an example. R. A. Van Nordstrand

C A.

2

Nature of the hydrogen bond. N. D. Sokolov. *Doklady Akad. Nauk S.S.S.R.* **58**, 611-14(1947).— Theoretical analysis of the exchange force wave functions involved in the configuration analogous to that of the O—H . . O hydrogen bond, by use of the approx. solution with the aid of Slater's functions, indicates that the H atom possesses the optimum parameters for establishment of such a link. The calcd. shift of the OH vibration frequency is about 320 cm.$^{-1}$, which is within reasonable range of the observed 270–490 cm.$^{-1}$.
G. M. Kosolapoff

SOKOLOV, N. D.

PA 9/49T90

USSR/Physics
Rotators
Adsorption

Aug 48

"Natural Values and Sum State for a Semispherical Rotator," N. D. Sokolov, Moscow, 1 p

"Zhur Eksper i Teoret Fiz" Vol XVIII, No 8

States that simultaneously with theoretical computation of adsorption coefficients and absolute speeds of heterogenous reactions, it is necessary to calculate sum state of molecule, which is adsorbed on adsorbent surface, and at same time is able to revolve freely about the contact point. This type of

[redacted] 9/49T90

USSR/Physics (Contd)

Aug 48

molecule can be tracked as a semisperical rotator. Submitted 29 Mar 1948.

[redacted] 9/49T90

SOKOLOV, N. D.

USSR/Chemistry - Hydrogen, Bonds May 1948
Chemistry - Protons, Transfer of

"Hydrogen Bond and Processes of Proton Transfer," N. D. Sokolov, Inst Org Chem, Acad Sci USSR, 4 pp

"Dok Ak Nauk SSSR" Vol LX, No 5

Continuation of experiments first reported in "Dok Ak Nauk SSSR," Vol LVIII, 1947, which described methods for obtaining bond frequency of A....B. Presents functions similar to results obtained in first article, with which it is possible to obtain a satisfactory description of spectroscopic phenomena of hydrogen bond. Submitted by Academician A. N. Terenin 10 Mar 1948.

68T16

SOKOLOV, N. D.

PA 8/49T4

USSR/Chemistry - Hydrogen Ion, **Discharge of** Jul 48
Chemistry - Overvoltage

"The Dependency of the Speed of the Discharge of Ions of Hydrogen on the Overvoltage," N. D. Sokolov, 3½ pp

"Dok Ak Nauk SSSR" Vol LXI, No 1

As is well known, the speed of discharge of hydrogen ions on a cathode is given by the equation

$$\ln i = a + b\eta \equiv a + \frac{\alpha F}{RT}\eta,$$

where i is current density, η is overvoltage and F, R, T have the usual meaning. The usual value of the α constant is about 0.5. Sokolov deduces theoretical

8/49T4

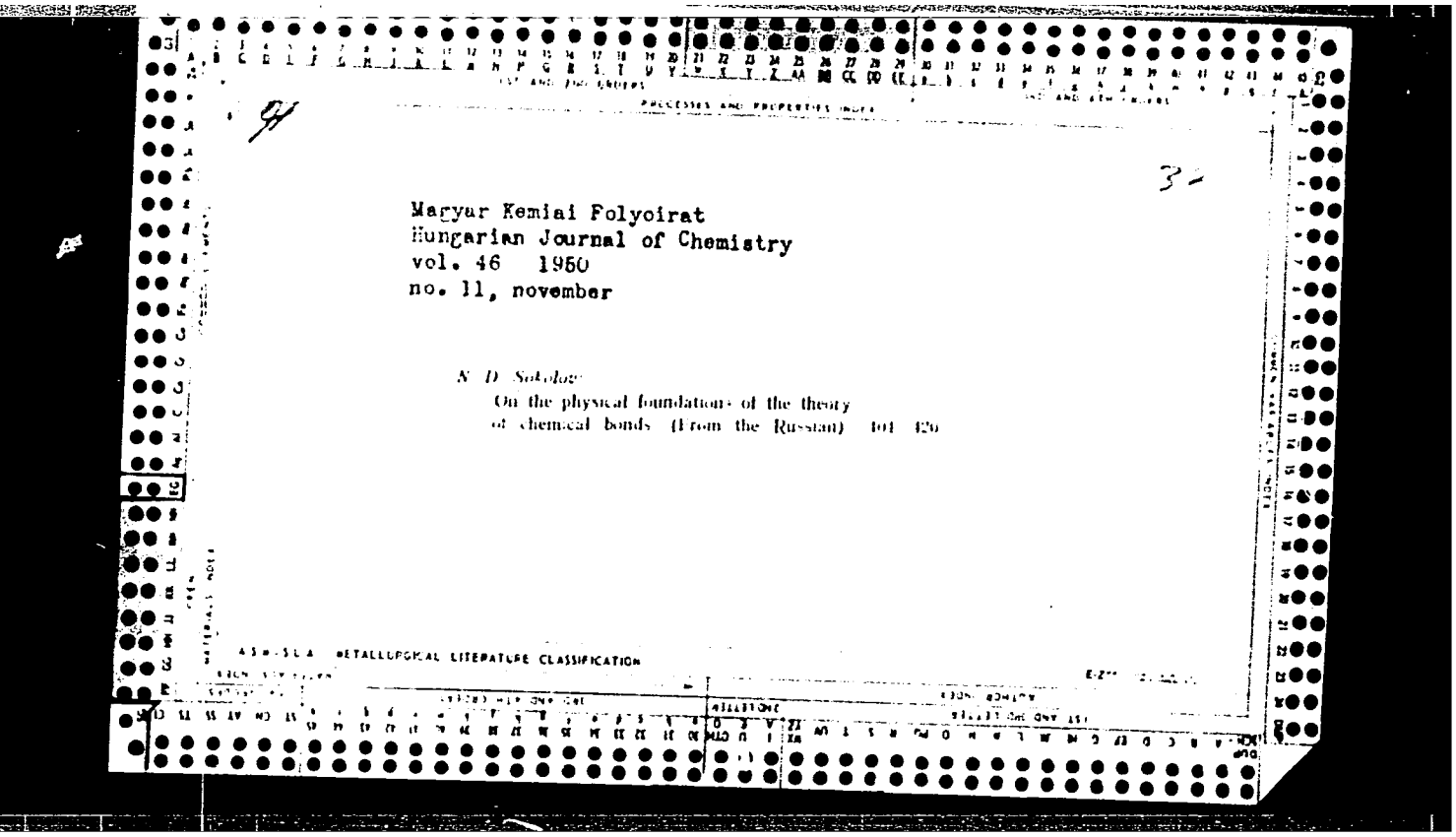
USSR/Chemistry - Hydrogen Ion, Discharge of (Contd) Jul 48

equation for α and shows that it gives results in conformity with experimental value. Submitted 14 Apr 1948.

8/49T4

CA

Physical bases of the theory of the chemical bond. N. D. Sokolov. *Uspekhi Khim.* 18, 697-723(1949).—A crit. review, involving in particular a criticism of Pauling's representation of resonance. 18 references. N. Thon



Magyar Kemiai Folyoirat
Hungarian Journal of Chemistry
vol. 46 1950
no. 11, november

N. D. Sokolov
On the physical foundations of the theory
of chemical bonds (From the Russian) 101 120

SOKOLOV, N.D., KURSANOV, D.N., KABACHNIK, M.I., KAVERZNEVA, Ye.D., PRILEZHAYEVA, Ye.N. and FREYDLINA, R. Kh.

"The Current State of Chemical Structure," Usp. Khim., 19, No.5, pp 529-544, 1950

Translation W-16104, 30 Dec 50

BUBEN, N. YA., VOYEVODSKIY, V. V., SOKOLOV, N. D.

Kondrat'yev, Victor Nikolayevich, 1900-

Scientific activities of V. N. Kondrat'yev. Usp. khim. 21 no. 8, 1952.

9. Monthly List of Russian Accessions, Library of Congress, November 1952 Uncl.

USSR/Physics - Quantum Mechanics Sep 52

"Quantum-Mechanical Treatment of the Interaction of a Polar Molecule With an Atom," N.D. Sokolov; Inst of Chem Phys, Acad Sci USSR

"Zhur Eksper i Teoret Fiz" Vol 23, No 3, pp 315-326

On the basis of the method of electron pairs, the author obtains an approx soln for the problem of interaction of a polar di-atomic mol with an atom possessing a filled external shell. The results are applied to the treatment of the hydrogen bond. Received 1 Aug 51.

227T87

SOKOLOV, N.D.

USSR

Theory of spectroscopic phenomena of the hydrogen bond. N. D. Sokolov. *Zhur. Eksptl. i Teoret. Fiz.* 23, 392–403(1952); *Science Abstr.* 56A, 726(1953); cf. *C.A.* 46, 5070f.—Among the unavoidable factors which det. the magnitude of the frequency shift is not only the dependence of z on R_{AH}; but also the lengthening of the bond A—H during formation of the system. This extension requires anharmonicity of vibrations. K. L. C.

Sokolov, N.D.

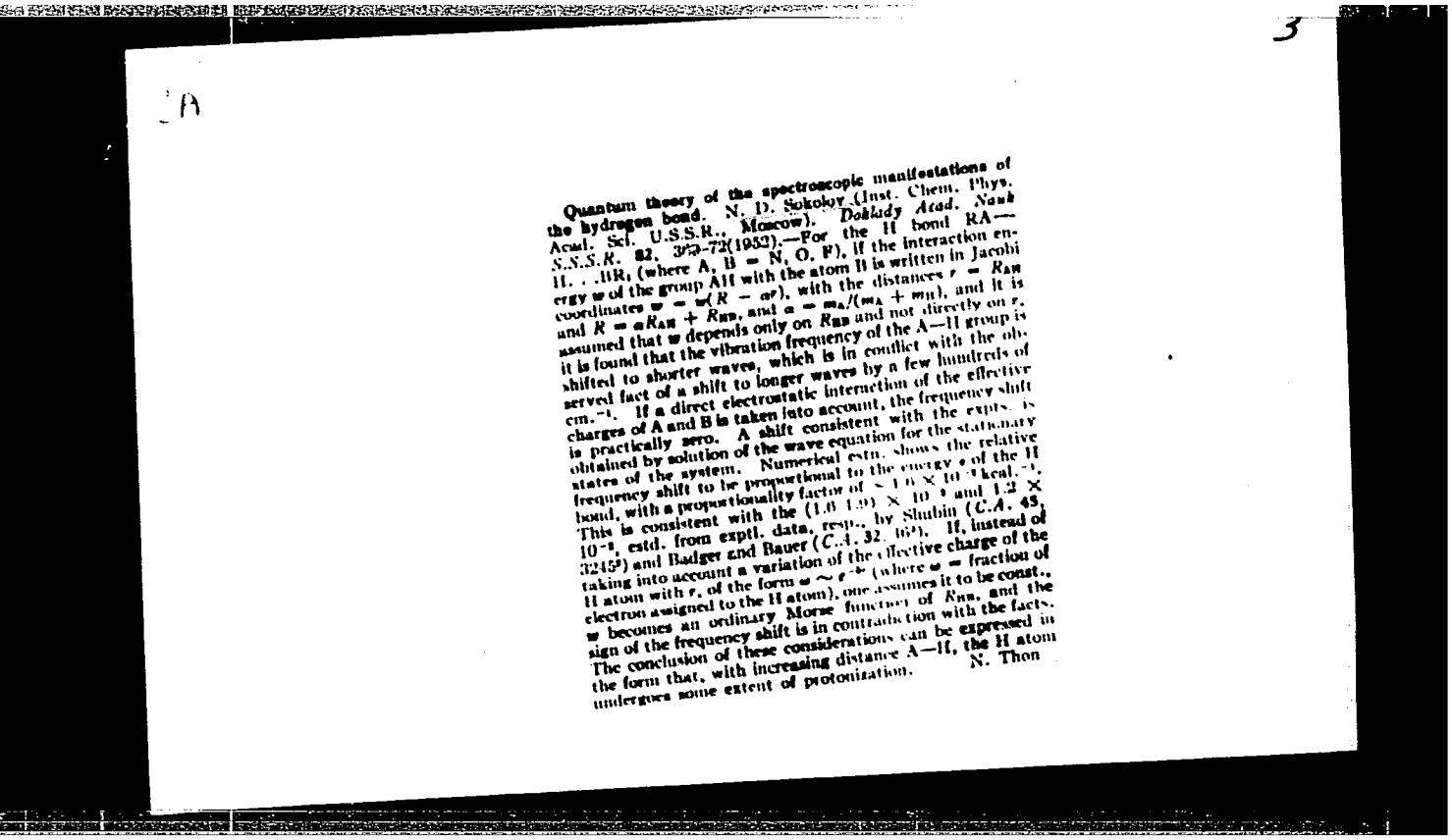
Chem

USSR

Quantum mechanical determination of the vibration frequencies of a compound with a hydrogen bond. N. D. Sokolov. *Zhur. Eksptl. i Teoret. Fiz.* 23, 401-11(1952); *Science Abstr.* 56A, 728-7(1953).—The vibration frequencies of the linear triat. system A—H...B with a H-bond were investigated. The most probable optical transition corresponds to a frequency differing little (~20%) from that obtained classically. An approx. proportionality exists between the A—H frequency shift under compd. formation and the energy of the H-bond. K. L. C.

SOKOLOV, N. D.

Quantum mechanical calculations of the deviations from the additivity scheme of organic chemistry. N. D. Sokolov (Inst. Chem. Phys., Acad. Sci. U.S.S.R., Moscow). *Zhur. Fiz. Khim.* 26, 1036–9(1952).—The additivity scheme of org. chemistry (cf. Syrkin, *C.A.* 36, 393[1]) which has been developed for satd. and ethylene hydrocarbons does not hold for aromatic compds. or those having a conjugated bond. In the latter cases the true heats of formation are usually higher than are those calcd. by the additive scheme. The deviation from this system has been calcd. by the methods of quantum mechanics. Only the π electrons are taken into account in the calcns., and the calcns. are carried out with a precision of some empirical factor. This factor appears to be almost const. for different mols. This is true for both the method of electron pairs and the method of mol. orbitals. J. Rovtar Leach



3

A

Quantum theory of the spectroscopic manifestations of the hydrogen bond. N. D. Sokolov (Inst. Chem. Phys. Acad. Sci. U.S.S.R., Moscow). *Doklady Akad. Nauk S.S.S.R.* 82, 389-92(1952).—For the H bond RA—H . . . BR$_1$ (where A, B = N, O, F), if the interaction energy w of the group AH with the atom B is written in Jacobi coordinates $w = w(R - \alpha r)$, with the distances $r = R_{AH}$ and $R = aR_{AH} + R_{HB}$, and $\alpha = m_A/(m_A + m_H)$, and it is assumed that w depends only on R_{HB} and not directly on r, it is found that the vibration frequency of the A—H group is shifted to shorter waves, which is in conflict with the observed fact of a shift to longer waves by a few hundreds of cm.$^{-1}$. If a direct electrostatic interaction of the effective charges of A and B is taken into account, the frequency shift is practically zero. A shift consistent with the expts. is obtained by solution of the wave equation for the stationary states of the system. Numerical estn. shows the relative frequency shift to be proportional to the energy ϵ of the H bond, with a proportionality factor of $\sim 1.0 \times 10^{-4}$ kcal.$^{-1}$. This is consistent with the (1.0-1.9) $\times 10^{-4}$ and 1.2×10^{-4}, estd. from exptl. data, resp., by Shubin (*C.A.* 45, 3245^g) and Badger and Bauer (*C.A.* 32, 169^1). If, instead of taking into account a variation of the effective charge of the H atom with r, of the form $w \sim e^{-br}$ (where w = fraction of electron assigned to the H atom), one assumes it to be const., w becomes an ordinary Morse function of R_{HB}, and the sign of the frequency shift is in contradiction with the facts. The conclusion of these considerations can be expressed in the form that, with increasing distance A—H, the H atom undergoes some extent of protonization. N. Thon

SOKOLOV, N. D.

Defended his Dissertation for Doctor of Physicomathematical Sciences, Leningrad State University, Leningrad, 1953.

Dissertation: "Intermolecular Reactions and Processes of Proton Transition"

SO: Referativnyy Zhurnal Khimiya, No. 1, Oct. 1953 (W/29955, 26 Apr 54)

Sokolov N.D.

TERENIN, A.N., akademik; KONDRAT'YEV, V.N., akademik; KNUNYANTS, I.L., akademik; KABACHNIK, M.I.; SOKOLOV, N.D., doktor fiz.-mat. nauk; REUTOV, O.A., doktor khimicheskikh nauk; MOSKVICHEVA, N.I., tekhnicheskiy redaktor

[Status of the theory of chemical structure in organic chemistry] Sostoianie teorii khimicheskogo stroeniia v organicheskoi khimii. Moskva, Izd-vo Akademii nauk SSSR, 1954. 122 p. [Microfilm] (MLRA 7:10)

1. Chlen-korrespondent AN SSSR (for Kabachnik) 2. Akademiya nauk SSSR. Otdeleniye khimicheskikh nauk

(Chemical structure) (Chemistry, Organic)

VOL'KENSHTEYN, M.V.; SOKOLOV, N.D., professor, redaktor; ESHMAN, Yu.A. redaktor; SMIRNOVA, A.V., tekhnicheskiy redaktor.

[Molecules and their structure] Molekuly i ikh stroenie. Moskva, Izd-vo Akademii nauk SSSR, 1955. 229 p. (MLRA 8:12)
(Molecules)

AF701597 TREASURE ISLAND BOOK REVIEW AID 809 - S

SOKOLOV, N. D., (Institute of Chemical Physics)
O VOZMOZHNOY ROLI DONORNO-AKTSEPTORNOY SVYAZI V GETEROGENNOM KATALIZE
(The potential role of the donor-acceptor bond in heterogeneous catalysis).
In Problemy kinetiki i kataliza (Problems of Kinetics and Catalysis), vol. 8. Izdatel'stvo Akademii Nauk SSSR, 1955. Section II: General problems of the theory of catalysis. p. 141-144.

The adsorption of molecules by solids might be explained by a donor-acceptor bond, i.e., as a result of the "polarization" of the molecule-"donor" in a positive -ion field or an atom (with a positive charge) of a molecule (crystal). However, there are few experimental data confirming the adsorption of molecules by means of donor-acceptor interaction. (A. N. Terenin's work on spectra of ammonia, some amines and other substances adsorbed by heteropolar crystals). There are several papers dealing with the theory of catalysis in which it is assumed that donor-acceptor bonds are formed in various stages of chemical transformations. The quantum - mechanism treatment of the donor-acceptor bond leads to the conclusion that the energy of the bond depends on the parameters which characterize the state of the non-shared electrons. The elucidation of the donor-acceptor mechanism should be confirmed experimentally, namely by studying spectra of adsorbed molecules and the poisoning of catalysts by impurities known to be absorbed with the aid of the donor-acceptor bond. 9 refs., 6 Russian (1929-1953).

1/1

SOKOLOV, N.D.

Possible role of the donor-acceptor bond in heterogeneous catalysis.
Probl.kin.i kat. 8:141-144 '55. (MLRA 9:5)

1. Institut khimicheskoy fiziki AN SSSR.
(Catalysis)

The hydration heat of atoms. V. N. Kondrat'ev and N. D. Sokolov (Inst. Chem. Phys., Acad. Sci. U.S.S.R., Moscow). *Zhur. Fiz. Khim.* 29, 1266–72(1955).—A system of relative heats of ion hydration is proposed, based on the universally accepted system of heat of formation of ions in soln., in which the heat of formation of the H ion in a dil. soln. is equated to 0. The heats of hydration of some alkoxy ions were calcd. on the basis of the relation between the hydration heats of the ions and their radii; also the affinity of the simplest alc. mol., to protons, etc. W. M. S.

Sokolov, N.D.

The hydrogen bond; N. D. Sokolov. *Uspekhi Fiz. Nauk* 57, 205–78(1955).—A review covering the exptl. and theoretical work on the H bond including its appearance in vibration, electron, and magnetic spectra. 139 references. J. Rovtar Leach

CH

SOKOLOV, N.D.

Hydrogen bond in proton transfers. Ukr. khim.zhur. 22 no.1:18-22 '56. (Hydrogen) (Protons) (MLRA 9:6)

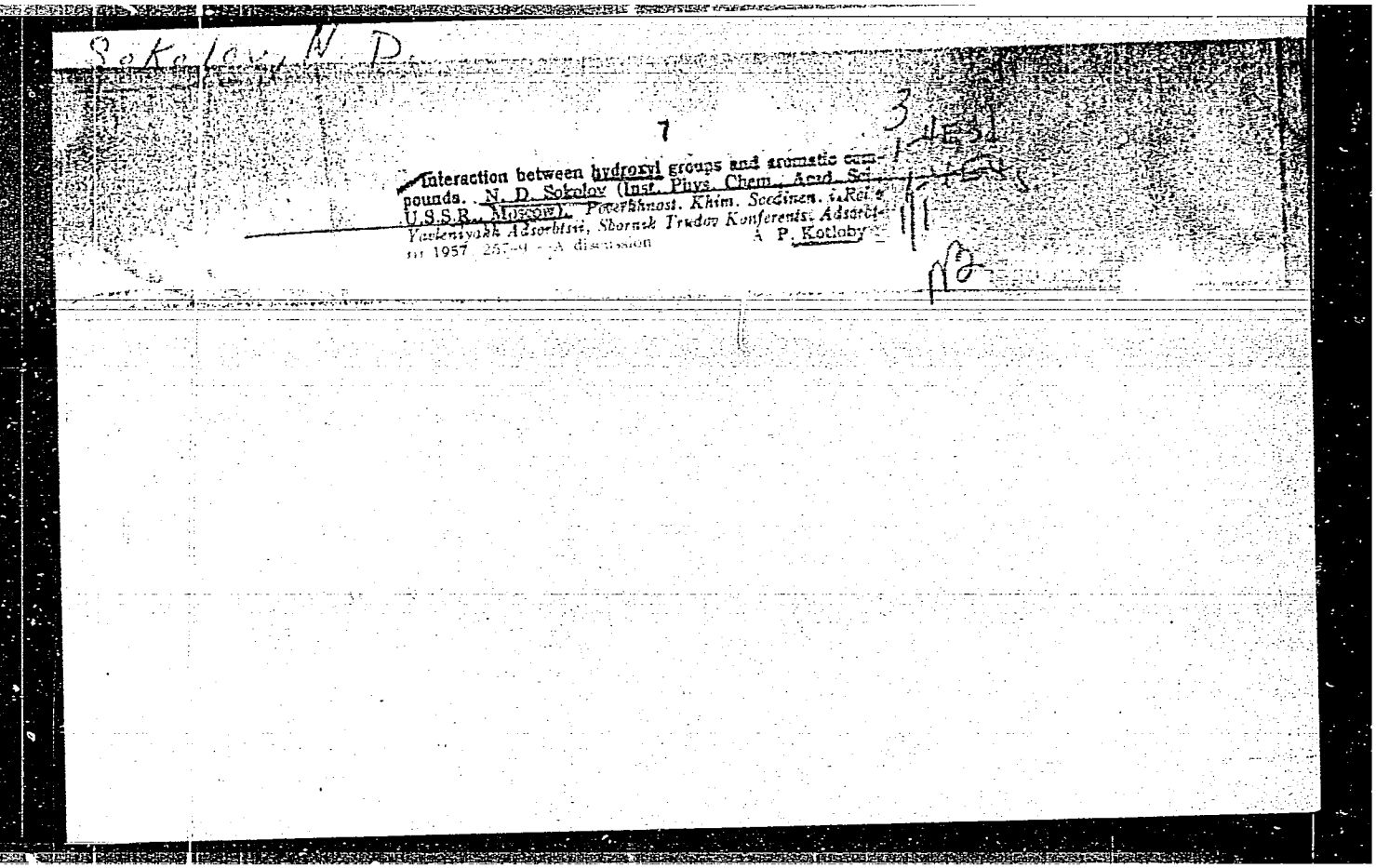
SOKOLOV, N.D.

2294. CORRELATION OF NUCLEAR QUADRUPOLE INTERACTION FREQUENCIES WITH POLAROGRAPHIC HALF-WAVE POTENTIALS. T. Iredale. Nature (London), Vol. 177, 36-7 (Jan. 7, 1956). 539.132

2295. THE HYDROGEN BOND. N.D.Sokolov. Uspekhi fiz. Nauk, Vol. 57, No. 2, 205-78 (1955). In Russian. 539.132

A survey article by the leading Soviet worker in the field. Among topics discussed are the following:- vibration spectra, the inadequacy of the simple electrostatic conception of the H-bond, quantum-mechanical treatment, calculation of the vibration frequency of an AH group in a complex with a hydrogen bond, the origin of the band in the vibration spectrum of an H-bond, electric and magnetic spectra, H-bond and proton transition processes. 139 refs.

C.R.S.Manders



Sokolov N. D.

7

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1453

Interaction between hydroxyl groups and aromatic compounds. N. D. Sokolov (Inst. Phys. Chem., Acad. Sci. U.S.S.R., Moscow). *Poverkhnost. Khim. Soedinen. i Ikh Vzaimodeistvie, Sbornik Trudov Konferentsii Adsorbtsii*, 1957. 257-9. — A discussion A. P. Kotloby

SOKOLOV N.D.

51-5-26/26

AUTHOR: Sokolov, N.D.

TITLE: Letter to the Editor: On the Article of V.M.Chulanovskiy and M.P.Burgova "On Inter-molecular Interaction in Solutions of Chloroform and Bromoform", II." (Ref.1)
(Pis'mo v redaktsiyu. Po povodu stat'i V.M.Chulanovskogo i M.P. Burgovoy "O mezh-molekulyarnom vzaimodeystvii v rastvorakh khloroforma i bromoforma. II")

PERIODICAL: Optika i Spektroskopiya, 1957, Vol.2, Nr 5, p.680 (USSR)

ABSTRACT: This is a complete translation. In using an arbitrary model of a hydrogen bond A-B...C (B = hydrogen atom) it is necessary for the energy of the system to be minimum at $r = r'_0$ and $R = R_0$. If this condition is not satisfied then one can obtain any result one wants to. From the basic equation in the article of V.M.Chulanovskiy and M.P. Burgova (Ref.1) $F(r, R-r) = F(r)-f(r) - \varphi(R-r)$ it follows that this condition is not obeyed, since $\varphi(R-r)$ includes only force of attraction between the atoms B and C but it does not contain the mutual repulsion of the latter and neglects the interaction between A and C altogether. For these reasons, therefore, the system A-B...C is unstable. Thus the authors' conclusions leading in particular to the correct dependence of the frequency displacement ($\Delta\nu$) on

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51-5-26/26

Letter to the Editor: On the Article of V.M.Chulanovskiy and M.P.Bumgova "On Inter-molecular Interaction in Solutions of Chloroform and Bromoform.II".

the increase of the equilibrium length of the bond A-B (Ref. 2,3) do not prove anything. It is shown (Ref.2,3) that if the condition of equilibrium is taken into account in the expression for the energy [i.e., in $\varphi(R-r)$ the repulsive force between B and C is included] then the frequency displacement is the reverse of that obtained experimentally. It is also shown that when the direct interaction of A and C is taken into account, then the value of $\Delta\nu$ is obtained with a correct sign but it is one order smaller than the experimental value. These results are not paradoxical as the authors of Ref.1 think, but they only mean (Ref.2,3) that an arbitrary model of a hydrogen bond which leads to expressions for the energy similar to, say, those given by an electrostatic model, is insufficient to explain the frequency displacement of the group AB (OH) in formation of this bond. Successful results are only possible by using quantum mechanics (Ref.2 to 4) which leads to more complicated dependence of the energy on interatomic distances in the system A-B...C and makes it possible to find the factors which cause the frequency displacement. The calculations show that the

Card 2/3

SOKOLOV, N. D.

VAYNSHTEYN, L.A., kandidat fiziko-matematicheskikh nauk; SOKOLOV, N.D., doktor fiziko-matematicheskikh nauk.

Theoretical spectroscopy and quantum mechanics of molecules. (Conference in Moscow). Vest. AN SSSR 27 no.6:101-104 Je '57. (MIRA 10:7)

(Quantum theory--Congresses) (Spectrum, Molecular)

SOKOLOV, N.D.,

"On the Quantum Theory of the Hydrogen Bond," paper submitted at IUPAP Symposium on Nature of Hydrogen Bonding, Ljubljana, Yugoslavakis, 30 July - 3 Aug 57.

Trans. Encl. B-3,096,177, 20 Jan 58.

also in Vestnik AN SSSR, 1957, Vol. 27, Nr. 11, pp. 137-139, "An Intl. Symposium on the Hydrogen Bond in Ljubljana." by Vol'kenshteyn, M. V.

SOKOLOV, N.D.

Relation between activation energy and the heat of reaction.
Dokl. AN SSSR 112 no.4:710-713 F '57. (MLRA 10:4)

1. Institut khimicheskoy fiziki Akademii nauk SSSR. Predstavleno akademikom V. N. Kondrat'yevym.
(Chemical reaction, Heat of)
(Activity coefficients)

Sokolov, N. D.

KUBAREV, S. I. and SOKOLOV, N. D.

"On the Theory of Dependence of Molecular Spectra on Intermolecular Interaction."

report presented at the 4th International Meeting of Molecular Spectroscopy, Bologna, Italy, 7-12 Sept 1959.

Moscow State University, Moscow, USSR.

21(1), 24(7) SOV/51-6-5-25/34

AUTHORS: Glasko, V.B., Maslov, V.P., Panikar, V.I. and Sokolov, N.D.

TITLE: On the Type of Correlation Function for the Helium Atom (O vide korrelyatsionnoy funktsii dlya atoma geliya)

PERIODICAL: Optika i Spektroskopiya, 1959, Vol 6, Nr 5, pp 698-700 (USSR)

ABSTRACT: In molecular calculations correlation in the motion of electrons is allowed for by introducing into the wave-function an additional factor dependent on inter-electron distance r_{ij} (Ref. 1).
In analogy with the first approximation in the helium atom calculations, carried out by Hylleraas (Ref 2), this multiplier can be written for a two-electron system in the form

$$f(r_{12}) = 1 + \alpha r_{12} \qquad (1)$$

where α is a variational parameter. In the general case the correlation function should depend on three correlation variables and f can be then represented as a series in powers of these variables (Refs 2, 3). When only one correlation variable is used the choice of the function $f(r_{12})$ in the form given by Eq (1) is an arbitrary one. The question arises as to whether this choice is the best possible one. This question is answered by determining the correlation function $f(r_{12})$ for the helium

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On the Type of Correlation Function for the Helium Atom

atom by a variational method. The result is shown as curve I in a figure on p 700; curve II represents the Hylleraas function given by Eq (1). Both curves are plotted as functions of distance in atomic units. The figure shows clearly that the correlation function approximation in the form of Eq (1) is practically the best choice, at least for atoms. The paper is entirely theoretical. There are 1 figure and 6 references, 3 of which are Soviet, 1 English, 1 German and 1 mixed (Soviet, English and French).

SUBMITTED: November 29, 1958

SOV/76-33-3-4/41

5(4)
AUTHOR: Sokolov, N. D.

TITLE: On the Energy of Conjugation (Ob energii sopryazheniya)

PERIODICAL: Zhurnal fizicheskoy khimii, 1959, Vol 33, Nr 3, pp 534 - 542 (USSR)

ABSTRACT: It is proved that a molecule model in which only the π-electrons are taken into account for the purpose of clarifying the decrease in energy in connection with the formation of conjugate bonds is insufficient as according to this model an increase in energy would have to take place instead of a decrease in energy. This is the reason why in connection with the aforesaid effect it is necessary to consider also the σ-electrons apart from the π-electrons . The energy of interaction between two σ- bonds or one σ-bond and one π-bond - which are usually neglected in connection with calculations of the deviations from the additive scheme - are of the same order of magnitude as the energy of the interaction between two π-bonds. As one of the main factors causing a decrease in energy in connection with the formation of con-

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jugate bonds the fact is regarded that the energy of the covalent bond decreases in the case of interaction with the other bond or with the free electron of the adjacent atom. According to a simplified variant of the method of the valence structure (using the equation according to London (1)) the above effects are qualitatively worked out by means of the example of the transition from propane to propylene. In connection with the aforesaid it is possible to explain the decrease in energy which is used in the case of breaking of the C-H bond in the CH_3-group and which decreases in connection with the transition from propane to propylene to 18 kcal; i.e. the energy of interaction between the free electron and the π-bond C=C in allyl is smaller than in the case of the σ-bond C-H in propyl, as the π-bond is weaker than the σ- bond. There are 2 figures and 14 references, 8 of which are Soviet.

ASSOCIATION: Akademiya nauk SSSR, Institut khimicheskoy fiziki Moskva (Academy of Sciences, USSR, Institute of Chemical Physics Moscow)

SUBMITTED: August 16, 1956

5 (4)

AUTHORS: Vetchinkin, S. I., Pshenichnov, Ye. A., Sokolov, N. D.

SOV/76-33-6-16/44

TITLE: Influence of the Hydrogen Bond on the Energy of the Ion Lattice of Ammonium Chloride and Evaluation of the Affinity of Ammonia Molecules to the Proton (Vliyaniye vodorodnoy svyazi na energiyu ionnoy reshetki khloristogo ammoniya i otsenka srodstva molekuly ammiaka k protonu)

PERIODICAL: Zhurnal fizicheskoy khimii, 1959, Vol 33, Nr 6, pp 1269-1274 (USSR)

ABSTRACT: It may be assumed that in ion crystals containing H_3O^+ or NH_4^+ ions, between cation and anion beside the Coulomb forces there is a hydrogen bond which increases the stability of the ion lattice. Usually, in energy computations this hydrogen bond is not considered (e.g. reference 1), which leads to a lesser result in computations of ion lattice energy. If, however, the exact ion lattice energy (IE) is known, the important molecular constant - the proton affinity (P) of the molecule - may be computed according to equation (1). The recently obtained value of Ref 3 for the (P) of the water molecule

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is lower by 19 kcal as compared to the value obtained according to Ref 2 , which points to the fact that in the computations per (Ref 3) the effect of the hydrogen bond between cation and anion was neglected. From quantum-mechanical computations (Ref 5) of the energy of interaction of the molecule A - H with the atom B (which exhibits an undivided electron pair) the following equation was derived: $W = Q + P_1\omega - P_2$ (2) (Q = Coulomb energy, $P_1\omega$ = repulsive energy between H and B, P_2 = exchange (or donor-acceptor) energy of the attraction between H and B). An investigation is then made of the applicability of equation (2) to the computation of interaction between the cation NH_4^+ and anion Cl^- in the NH_4Cl crystal and it was found that by the selected semiempirical computation method a computation is possible only if $P_2 = 0$ is assumed, by which a lower (IE) is obtained. The change of the (IE) caused by the hydrogen bond is assumed to be of the

same magnitude as the last mentioned decrease in the (IE). From this point of view a computation of the lattice energy for ammonium chloride is made and it is found that the correction of the computation according to Bleick (Ref 1), in which the hydrogen bond was neglected, must be of the magnitude 10 kcal, and, consequently, the value $P_{NH_3} = 194 \pm 7$ kcal. There are 1 figure, 1 table, and 10 references, 7 of which are Soviet.

ASSOCIATION: Akademiya nauk SSSR, Institut khimicheskoy fiziki, Moskva (Academy of Sciences of the USSR, Institute of Chemical Physics, Moscow)

SUBMITTED: October 31, 1957

5(4)
AUTHORS: Aleksandrov, I. V., Sokolov, N. D. SOV/20-124-1-32/69

TITLE: The Hydrogen Bond and Proton Magnetic Resonance (Vodorodnaya svyaz' i protonnyy magnitnyy rezonans)

PERIODICAL: Doklady Akademii nauk SSSR, 1959, Vol 124, Nr 1, pp 115-118 (USSR)

ABSTRACT: The dependence of the shielding of a proton upon the degree of the polarity of the A-H-bond can be estimated according to a method suggested by I. V. Aleksandrov (Refs 10, 11). If, as a wave function, the molecular path composed of the 1s-function of the H-atom as well as of the 2s- and 2p-Slater functions of the O-atom is selected in the form $\psi^0 = N\left[\varphi_{1s} + \lambda(a\varphi^0_{2s} + b\varphi^0_{2p})\right]$, the parameter λ characterizes the degree of polarity of the bond O – H. The value of λ is near 1 and the constant σ of magnetic shielding can be determined as a function of λ. At the distance R = 1Å between the nuclei it holds with sufficient accuracy that $\Delta\sigma_1 = -1.5 \cdot 10^{-5}\Delta\lambda$. If λ increases by $\Delta\lambda = 0.3$ under the influence of the H-bond, it holds that $\Delta\sigma_1 \approx -4.5 \cdot 10^6$. The

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influence exercised by expansion of the O-H-bond can be estimated by means of the same formulas as the influence exercised by polarity. For small variations of R in the case of $\lambda = 1$ it holds that $\Delta\sigma_2 = - k. 10^{-5}\Delta R.$ At $\Delta R = 0.05$ Å one finds $\Delta\sigma_2 \sim -0.5. 10^{-6}$. The influence of the donor-acceptor bond $H^+.....O$ can be approximately taken into account if the molecular orbit of this bond is represented in the form $\psi = N' (\varphi_{2p} + \beta\varphi_{1s})$. If the inter-atomic distance H.....O is 1.7 Å, the contribution of this bond made towards magnetic shielding of the proton amounts to $\Delta\sigma_3 = (-0.08 + \beta + 3.6\beta^2). 10^{-5}$, and with $\beta \approx 0.2$ there follows $\Delta\sigma_3 \approx + 2.5. 10^{-6}$. If an electric field is applied σ varies by $\Delta\sigma_4 = -(5a_o^3/mc^2) E^2$, where a_o denotes the Bohr radius. The influence exercised by the second not filled electron pair (the cloud of which has an axis which is vertical to the line H....O) of the O-atom is taken into account by the formula

$\Delta\sigma_5 = \frac{\chi - \chi_{zz}}{R^3}$, where χ_{zz} denotes the zz-component of the diamagnetic susceptibility χ. In the case of R = 1.7 Å, $\Delta\sigma_5$ is in the interval of from + 0.2. 10^{-6} to -0.2. 10^{-6}. The data concerning the magnetic shielding of the proton in the H-bond confirm, firstly, the hypothesis that the polarity of the A-H-bond increases considerably by the formation of an H-bridge and, secondly, they agree with the hypothesis of the formation of the donor-acceptor-bond AH....B. There are 11 references, 3 of which are Soviet.

ASSOCIATION: Institut khimicheskoy fiziki Akademii nauk SSSR (Institute for Chemical Physics of the Academy of Sciences, USSR)

PRESENTED: July 28, 1958, by V. N. Kondrat'yev, Academician

SUBMITTED: July 23, 1958

5(4), 24(7) SOV/20-124-2-35/71

AUTHORS: Nikitin, Ye. Ye., Sokolov, N. D.

TITLE: On the Relation Between the Dissociation Constants of the Thermal Docomposition of Biatomic Molecules in the Presence and in the Absence of Equilibrium (O sootnoshenii mezhdu konstantami skorosti termicheskogo raspada dvukhatomnykh molekul pri nalichii i pri otsutstvii ravnovesiya)

PERIODICAL: Doklady Akademii nauk SSSR, 1959, Vol 124, Nr 2, pp 366-369 (USSR)

ABSTRACT: Short reference is first made to earlier papers on the dissociation of biatomic molecules AB + M $\longrightarrow$ A + B + M. The disturbance of Boltzmann distribution over the oscillation states of the decomposing molecule decreases the degree of population of the oscillation levels near the limit of dissociation. The disturbance of Boltzmann distribution increases as a result of the decrease of the oscillation quanta near the limit of dissociation. The kinetics of thermal decomposition and of recombination probably does not satisfy the usual kinetic equation. Dissociation is a process developing in several stages and therefore the kinetics of decomposition and recombination

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On the Relation Between the Dissociation Constants of the Thermal Decomposition of Biatomic Molecules in the Presence and in the Absence of Equilibrium

must be described by the following systems of equations: $(d/dt)x_n = -\sum_k P_{nk}x_n + \sum_k P_{kn}x_k$. Here x_n denotes the distribution function, i.e. the degree of population of the n-th level of the system AB, and P_{kn} - the probabilities of the rotation- and oscillation transitions $k \longrightarrow n$ of the molecule AB. The sums of the formula given above extend also to states of the continuous part of the spectrum. The authors investigate the simplest case in which at $[AB] \ll [M]$ the concentrations $[A]_o$ and $[B]_o$ are kept constant. The aforementioned system of equations becomes linear and can be written down in the form $(d/dt)\hat{X} = \hat{B}\hat{X} + \hat{C}[A]_o[B]_o$. The only column of the matrix $\hat{X}$ is composed of the components of the distribution function x_n, and the matrices $\hat{B}$ and $\hat{C}$ describe the successive decomposition and recombination respectively. An expression is then written down for the general solution of the last-mentioned equation.

On the Relation Between the Dissociation Constants of the Thermal Decomposition of Biatomic Molecules in the Presence and in the Absence of Equilibrium

The first eigenvalue of the matrix $-\hat{B}$ corresponds to the dissociation-constant of decomposition and is, in the case of lacking recombination, determined by the expression $\mu_o = -(d/dt)\,[AB] \,/\, [AB]$. The second eigenvalue μ_1 of the matrix $-\hat{B}$ is approximately equal to the rate of relaxation of the oscillation energy of the molecule AB, where, by the way, $\mu_o \ll \mu_1$ holds. The solution of the equation $\hat{B}\hat{X}_o + \hat{C}[A]_o[B]_o = 0$ is the distribution function $x_n^{(o)} = N \exp(-E_n/kT)$ corresponding to equilibrium. Next, the amount of the constant N is determined, after which an equation is written down for the kinetics of thermal decomposition and of recombination. In the case of equilibrium the dissociation constant of decomposition is greater than the dissociation constant k_d in the case of lacking equilibrium. The calculated values of k_d for the thermal decomposition of J_2, Br_2 and O_2 agree satisfactorily with the

On the Relation Between the Dissociation Constants of the Thermal Decomposition of Biatomic Molecules in the Presence and in the Absence of Equilibrium

values which were determined experimentally by the kinetic method in the decomposition of molecules in the shock wave in an argon atmosphere at temperatures of 1500 - 4000° K. The dissociation constant corresponding to equilibrium is greater by one order of magnitude than the value corresponding to the lacking equilibrium. There are 15 references, 5 of which are Soviet.

ASSOCIATION: Institut khimicheskoy fiziki Akademii nauk SSSR (Institute for Chemical Physics of the Academy of Sciences, USSR)

PRESENTED: August 7, 1958, by V. N. Kondrat'yev, Academician

SUBMITTED: July 11, 1958

S/051/60/008/04/025/032
E201/E691

AUTHORS: Aleksandrov, I.V., Korst, N.N. and Sokolov, N.D.

TITLE: The Effect of the Mobility of Protons on the Width of Nuclear Magnetic Resonance Lines in Crystals

PERIODICAL: Optika i spektroskopiya, 1960, Vol 8, Nr 4, pp 575-577 (USSR)

ABSTRACT: The mobility of hydrogen atoms (protons) in condensed phases may be due to internal rotation or translational transitions from one equilibrium position to another. Nuclear magnetic resonance of protons is one of the most effective methods of investigation of their mobility. The present notedescribes how the second moment of the nuclear magnetic resonance signal of protons in ice can be used to find the mechanism of proton transitions. The paper is entirely theoretical. There are 6 references, 5 of which are English and 1 from Acta Crystallographica.

SUBMITTED: October 10, 1959

Card 1/1

Theory of the Thermal Decay of Diatomic Molecules

than D. By integrating (8), an additional pre-exponential factor appears. The non-equilibrium distribution function corresponding to the exponential decay is determined by the first eigenvector $l_n(\mu_o)$ of the matrix B. $l_n(\mu_o)$ can be easily found from the general formulas of the eigenvectors of the Jacobian matrix if the formula for μ_o is known. The percentual improvement in population of the upper vibration levels is of the order of $\exp[(D - E_p)/kT]$, where p is the number of vibration levels calculated from the dissociation limit. This result especially corresponds to Refs. 9 and 13 dealing with the model of a decaying harmonic oscillator. Since in the case of a real anharmonic oscillator the oscillation quanta at the dissociation limit are small compared with kT, numerous levels reach the region of great improverishment $D - E_p \approx kT$. Hence, it may be said that the equilibrium of the Boltzmann distribution in decay reactions is always perturbed. Since dissociation is a complex multistage process, the quantity K_d becomes small compared with the quantity obtained from the equilibrium condition $(K_d)_{equil} = KK_{rec}$ owing to the perturbation of the

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S/058/61/000/011/005/025
A058/A101

AUTHORS: Aleksandrov, I.V., Korst, N.N., Sokolov, N.D.

TITLE: Proton exchange effect on nuclear magnetic resonance line width in crystals

PERIODICAL: Referativnyy zhurnal. Fizika, no. 11, 1961, 126, abstract 11V221 (V sb. "Paramagnitn. rezonans", Kazan', Kazansk. un-t, 1960, 186 - 188)

TEXT: The authors calculate the second moment of the nuclear magnetic resonance line in ice crystals. They show that incident to proton tunneling along the hydrogen bonds the second moment decreases by $\sim$ 20% (on condition that the tunneling frequency is appreciably greater than the nuclear magnetic resonance line width).

I. Aleksandrov

[Abstracter's note: Complete translation]

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PSHENICHNOV, Ye.A.; SOKOLOV, N.D.

Quantum effects in a double potential well and spectroscopy of the hydrogen bond. Opt.i spektr. 11 no.1:16-23 Jl '61. (MIRA 14:10)

(Hydrogen bonding) (Quantum theory) (Spectrum analysis)

VETCHINKIN, S.I.; SOKOLOV, N.D.

Calculation of the system HeH^+ by means of the valence structure method. Zhur. fiz. khim. 35 no.7:1645-1647 Jl '61.
(MIRA 14:7)

1. AN SSSR, Institut khimicheskoy fiziki.
(Helium hydride)

PSHENICHNOV, Ye.A.; SOKOLOV, N.D.

Polanyi's law for proton transitions and the hydrogen bond. Dokl. AN SSSR. 137 no. 2:352-355 Mr '61. (MIRA 14:2)

1. Institut khimicheskoy fiziki AN SSSR i Moskovskiy gosudarstvennyy universitet im.M.V. Lomonoseva. Predstavleno akademikom V.N. Kondrat'yevym.

(Protons) (Hydrogen bonding)

FRISH, S.E., otv. red.; BOBOVICH, Ya.S., kand. fiz.-matem. nauk, red.; VOL'KENSHTEYN, M.V., doktor fiz.-matem. nauk, red.: GALANIN, M.D., doktor fiz.-matem. nauk, red.; DRUKAREV, G.F., doktor fiz.-matem. nauk, red.; YEL'YASHEVICH, M.A., akademik, red.; KALITEYEVSKIY, N.I., doktor fiz.-matem. nauk, red.; KUSAKOV, M.M., doktor khim. nauk, red.; LIPIS, L.V., doktor tekhn.nauk, red.; PEKAR, S.I., doktor fiz.-matem. nauk, red.; PROKOF'YEV, V.K., doktor fiz.-matem. nauk, red.; SOKOLOV, N.D., doktor fiz.-matem. nauk, red.; FEOFILOV, P.P., doktor fiz.-matem. nauk, red.; CHULANOVSKIY, V.M., doktor fiz.-matem. nauk, red.; SHPOL'SKIY, E.V., doktor fiz.-matem. nauk, red.; YAROSLAVSKIY, N.G., kand. fiz.-matem. nauk, red.; LEKSINA, I.Ye., red. izd-va; PENKINA, N.V., red. izd-va; NOVICHKOVA, N.D., tekhn. red.; KASHINA, P.S., tekhn. red.

[Physical problems in spectroscopy]Fizicheskie problemy spektroskopii; materialy. Moskva, Izd-vo Akad. nauk SSSR, Vol.1. 1962. 474 p. (MIRA 16:2)

1. Soveshchaniye po spektroskopii. 13th, Leningrad, 1960. 2. Chlen-korrespondent Akademii nauk SSSR (for Frish). 3. Akademiya nauk Belorusskoy SSR (for Yel'yashevich).
(Spectrum analysis)

SOKOLOV, N.D.

35065

S/195/62/003/001/006/010
E071/E136

5.1115

AUTHORS: Kvlividze, V.I., Iyevskaya, N.M., Yegorova, T.S., Kiselev, V.F., and Sokolov, N.D.

TITLE: NMR studies of water vapour adsorption on the surface of silica gel

PERIODICAL: Kinetika i kataliz, v.3, no.1, 1962, 91-98

TEXT: The mechanism of adsorption and the state of the adsorbed molecules on the surface of an adsorbent cannot be elucidated on the basis of purely adsorptive measurement. For this purpose some additional data on the system adsorbed substance - adsorbent obtained by physical methods are necessary. As a first stage in the investigations the authors studied signals of nuclear magnetic resonance from protons of hydroxyl groups of water adsorbed on the surface of silica gel. The results obtained were compared with adsorption properties of silica gel, with measurements of heats of adsorption and available spectroscopic data. Silica gels K-2 (K-2) and K-4 (K-4) obtained by the hydrolysis of $SiCl_4$ and a purified sample of technical silica gel

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KCK-3 (KSK-3) were used for the investigation. The NMR measurements were carried out at room temperature on a sample of 0.2-0.3 g. The width of the lines was measured as the distance between maxima on the differential curve. The second moment was calculated from the differential curve of the signal absorption. Additions of water vapour in the ampule with silica gel for NMR and adsorption measurements were carried out by means of a spring balance. Heats of adsorption were determined either directly from calorimetric measurements or by the differentiation of the curve relating the heat of wetting and the amount of water adsorbed on the specimen. From the adsorption data and heat of wetting curves, differential curves of the changes in free energy and entropy of adsorption were calculated. It was shown that molecules of water are absent on the surface of the samples evacuated at 200 °C. In the initial stage of adsorption a sharp decrease in the width of the line of the second moment was observed. These changes in the NMR signals agree with the trends of the curves of differential heat and entropy of adsorption. The possibility of interaction of water molecules

with the surface of silica gel through the coordination and hydrogen bonds is discussed.
There are 5 figures and 1 table.

ASSOCIATION: Moskovskiy gosudarstvennyy universitet im. M.V. Lomonosova, Fizicheskiy fakul'tet (Moscow State University imeni M.V. Lomonosov, Physics Division)

SUBMITTED: July 3, 1961

S/030/62/000/010/006/007
D204/D307

AUTHOR: Sokolov, N. D., Doctor of Physico-Mathematical Sciences

TITLE: Investigations of the hydrogen bond

PERIODICAL: Akademiya nauk SSSR. Vestnik, no. 10, 1962, 110-112

TEXT: A summary is given of a symposium on the subject of the hydrogen bond, held in Leningrad over July 4 - 7, 1962, organized by the Fizicheskiy fakultet Leningradskogo universiteta (Physics Faculty of Leningrad University), the Nauchnnyy sovet (Scientific Council) concerned with the theories of chemical structure, kinetics, reactivity and catalysis, and by the Komissiya po spektroskopii Akademii nauk SSSR (Spectroscopy Commission of the Academy of Sciences, USSR), with the participation of over 200 scientists. The following topics were discussed: (1) The theory of the hydrogen bond; (2) Spectroscopy of the hydrogen bond (the most fully discussed subject during the symposium); (3) Structures of hydrogen-bonded compounds; (4) The nature of hydrogen bond in liquids

Card 1/2

KOKOLOV, M.D., doktor fiz.-matem.nauk

Problems of quantum chemistry. Vest. AN SSSR 32 no.9:135-138 S '62. (MIRA 15:9)

(Quantum chemistry)

VETCHINKIN, S.I.; SOKOLOV, N.D.

Calculation of molecular integrals in quantum chemistry. Zhur.fiz. khim. 36 no.8:1754-1756 Ag '62. (MIRA 15:8)

1. Institut khimicheskoy fiziki AN SSSR i Moskovskiy gosudarstvennyy universitet fizicheskiy fakul'tet.
(Quantum chemistry)

S/020/62/147/003/018/027
B104/B186

AUTHORS: Korst, N. N., Savel'yev, V. A., Sokolov, N. D.

TITLE: Consideration of the averaging over the natural vibrational state when calculating the second moment of the nuclear magnetic resonance signal

PERIODICAL: Akademiya nauk SSSR. Doklady, v. 147, no. 3, 1962, 594 - 596

TEXT: Neglecting the uncertainty of the position of the protons in their natural vibrational state leads to the difference between the second moments of the n.m.r. proton line of ice as calculated with the van Vleck formula, which was $\langle \Delta\omega^2 \rangle = 25$ gauss^2 for stationary protons (this value is lower by 20% when the protons perform a motion along the H-bonds) and those measured in experiments ($T = 90^\circ K$; $\langle \Delta\omega^2 \rangle = 36.7 \pm 1.7$ gauss^2; K. Kume, J. Phys. Soc. Japan, 15, 1493 (1960)). The uncertainty is associated with the zero energy of the atoms. With consideration of neighboring proton pairs, the second moment of an ice single crystal is

$$\langle \Delta\omega^2 \rangle = \frac{3}{4} g^4 \beta^4 \hbar^{-2} I (I+1) \left[\frac{3\cos^2\theta - 1}{R^3}\right]^2. \qquad (2).$$

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Expanding into powers of the deviations of the coordinates from their equilibrium values (after averaging over all possible mutual positions of the vectors $\vec{R}$ and $\vec{H}$) leads to

$$\langle \Delta\omega^2 \rangle = \frac{3}{5} g^4 \beta^4 \hbar^{-2} R^{-6} I (I+1) \left\{ 1 + \frac{6\overline{(\Delta r_1)^2}}{\left[2r_0 \sin\frac{\Phi_0}{2}\right]^2} + \frac{6\overline{(\Delta r_2)^2}}{\left[2r_0 \sin\frac{\Phi_0}{2}\right]^2} + \right.$$
$$\left. + \frac{10\,\overline{\Delta r_1 \Delta r_2}}{\left[2r_0 \sin\frac{\Phi_0}{2}\right]^2} + \frac{9}{4}\overline{(\Delta\Phi)^2} + \frac{87}{32}\overline{[(\Delta\Phi)^2]^2} \right\}, \qquad (3)$$

for a polycrystal. $\vec{R}_{ij}$ is the radius vector linking the i-th proton to the j-th. Computation with formula (3) showed that the term $\overline{(\Delta\phi)^2}$ makes up 70% of the correction to the second moment. Considering more distant protons one obtains

$$\langle \Delta\omega^2 \rangle = 0{,}80\,\gamma^4\hbar^2 R^{-6}\{1 + 0{,}21\} = 31{,}1 \quad \text{gauss}^2.$$

Further improvement can be achieved by taking the hydrogen bond into

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Consideration of the...

account. The results show that proton transitions along the hydrogen bonds at T = 90°K have little probability. Similar calculations of the second moments of polyethylene and of 1,2-dichloro ethane with formula (5) yielded good agreement with experimental data as published in J. Polym. Sci., 26, 171 (1957); J. Chem. Soc., 17, 972 (1949). There is 1 table.

ASSOCIATION: Fizicheskiy institut im. P. N. Lebedeva Akademii nauk SSSR (Physics Institute imeni P. N. Lebedev of the Academy of Sciences USSR)

PRESENTED: May 14, 1962, by V. N. Kondrat'yev, Academician

SUBMITTED: April 30, 1962

Card 3/3

SAVEL'YEV, V.A.; SOKOLOV, N.D.

Calculating the extension of the hydrogen bond in isotopic substitution in ice. Fiz. tver. tela 5 no.11:3273-3275 N '63. (MIRA 16:12)

1. Institut khimicheskoy fiziki AN SSSR, Moskva.

SZOKOLOV, N.D. [Sokolov, N.D.]

Quantum theory of the electron cloud of molecules. Magy fiz folyoir 11 no.2:159-176 '63.

SOKOLOV, N.D.

Symposium on hydrogen bonding. Opt. i spektr. 15 no.1:142-144 Jl '63. (MIRA 16:8)

(Hydrogen bonding)

SOKOLOV, N.D.

State and several problems of the theory of the electronic clouds of molecules. Usp.khim. 32 no.8:967-983 Ag '63. (MIRA 16:9)

1. Institut khimicheskoy fiziki AN SSSR.

SOKOLOV, N. D.

"Electron paramagnetic resonance" by S. A. Al'tshuler, B. M. Kozyrev. Reviewed by N. D. Sokolov. Usp. fiz. nauk 79 no.1: 165-166 Ja '63. (MIRA 16:1)

(Paramagnetic resonance and relaxation)
(Al'tshuler, S. A.) (Kozyrev, B. M.)

SOKOLOV, N. D.; KORST, N. N.; and SAVELYEV, B. A.

"Calculation of the Temperature-Dependence of Low Vibrational Frequencies in Ice."

papers presented by USSR and Polish Scientists at the VIIth European Congress on Molecular Spectroscopy (IUPAC), held 22-27 July 1963 in Budapest, Hungary.

SOKOLOV, N.D., prof., otv. red.; CHULANOVSKIY, V.M., prof., otv. red.; BUCHACHENKO, A.L., red.

[Hydrogen bonding] Vodorodnaia sviaz'; sbornik statei. Moskva, Izd-vo "Nauka," 1964. 339 p. (MIRA 17:8)

1. Akademiya nauk SSSR. Institut khimicheskoy fiziki.

ACCESSION NR: AP4028464 S/0181/64/006/004/1242/1243

AUTHORS: Korst, N. N.; Savel'yev, V. A.; Sokolov, N. D.

TITLE: The second moment of the NMR signal and the structure of ice

SOURCE: Fizika tverdogo tela, v. 6, no. 4, 1964, 1242-1243

TOPIC TAGS: nuclear magnetic resonance, second moment, ice structure

ABSTRACT: Magnitudes of the second moment $\langle \Delta\omega^2 \rangle$ of the NMR signal from the protons of ice are computed by the modified Van Vleck formula in which the uncertainty in proton position due to the zero vibrational energy is considered. The extreme values of the geometrical parameters are used: the length of the O-H bond in ice, r_0 (0.98Å and 1.01 Å) and the H-O-H valence angle, φ_0 (104° and 109°28'). Values for the second moment are obtained between 33 and 40 (gauss)^2, taking into account the frequency-temperature dependence and the exchange of protons by the tunnel effect. These values are not significantly different from the experimental value

$$\langle \Delta\omega^2 \rangle = 36.7 \pm 1.7 \text{ (gauss)}^2.$$

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ACCESSION NR: AP4028464

It is concluded that it is impossible to compute an exclusive model of ice in which there is an exchange of protons by random tunnelling. Orig. art. has: 6 equations.

ASSOCIATION: Institut khimicheskoy fiziki AN SSSR, Moscow (Institute of Physical Chemistry AN SSSR)

SUBMITTED: 25Nov63 DATE ACQ: 27Apr64 ENCL: 00

SUB CODE: PH NO REF SOV: 004 OTHER: 005

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SAVEL'YEV, V.A.; SOKOLOV, N.D.

Temperature dependence of the intermolecular vibration frequency in ice. Opt. i spektr. 17 no.1:35-37 Jl '64. (MIRA 17:9)

L 8758-65 EWT(1) IJP(c) ESD(t)/AEWL

ACCESSION NR: AP4044845 S/0051/64/017/003/0343/0348

AUTHOR: Pshenichnov, Ye. A.; Sokolov, N. D. 15

TITLE: Eigenvalues and probabilities of quantum transitions in a double asymmetrical potential well

SOURCE: Optika i spektroskopiya, v. 17, no. 3, 1964, 343-348

TOPIC TAGS: deuterated compound, quantum transition, proton transition, tunneling transition

ABSTRACT: The calculations were made for the A--D ... B bond, in analogy with the similar calculations made by R. L. Somorjai and D. F. Hornig (J. Chem. Phys., v. 36, 1980, 1962) for the A--H ... B bond. In addition to serving as a check on the characteristic features of a double asymmetrical well, the present calculations were aimed at improving the accuracy of the earlier ones, inasmuch as Somorjai and Hornig confined themselves only to the 20th order

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ACCESSION NR: AP4044845

(N = 20) of the corresponding secular equation, which is not accurate enough. The accuracy is all the more suspect because the calculations of Somorjai and Hornig also lead to the conclusion that the tunneling transition of the proton from one well to the other is more probable at ordinary temperatures than above-the-barrier transition. The authors have calculated the eigenvalues and the eigenfunctions for N = 30 for 4 variants of potential wells used by Somorjai and Hornig, using the electronic computer of the Mathematics Center of IKhF AN SSSR. The somewhat lesser attenuation of the oscillation intensity following substitution of deuterium for hydrogen, compared with the usual attenuation in free molecules, is used to conclude that a second potential well exists. It is noted in conclusion that the calculations make it possible to investigate the mechanism of the transition of a proton or a deuteron from one potential well to the other, and that this investigation will be reported by the authors in the journal "Kinetika i kataliz." Orig. art. has: 3 tables, 1 figure, and 2 formulas.

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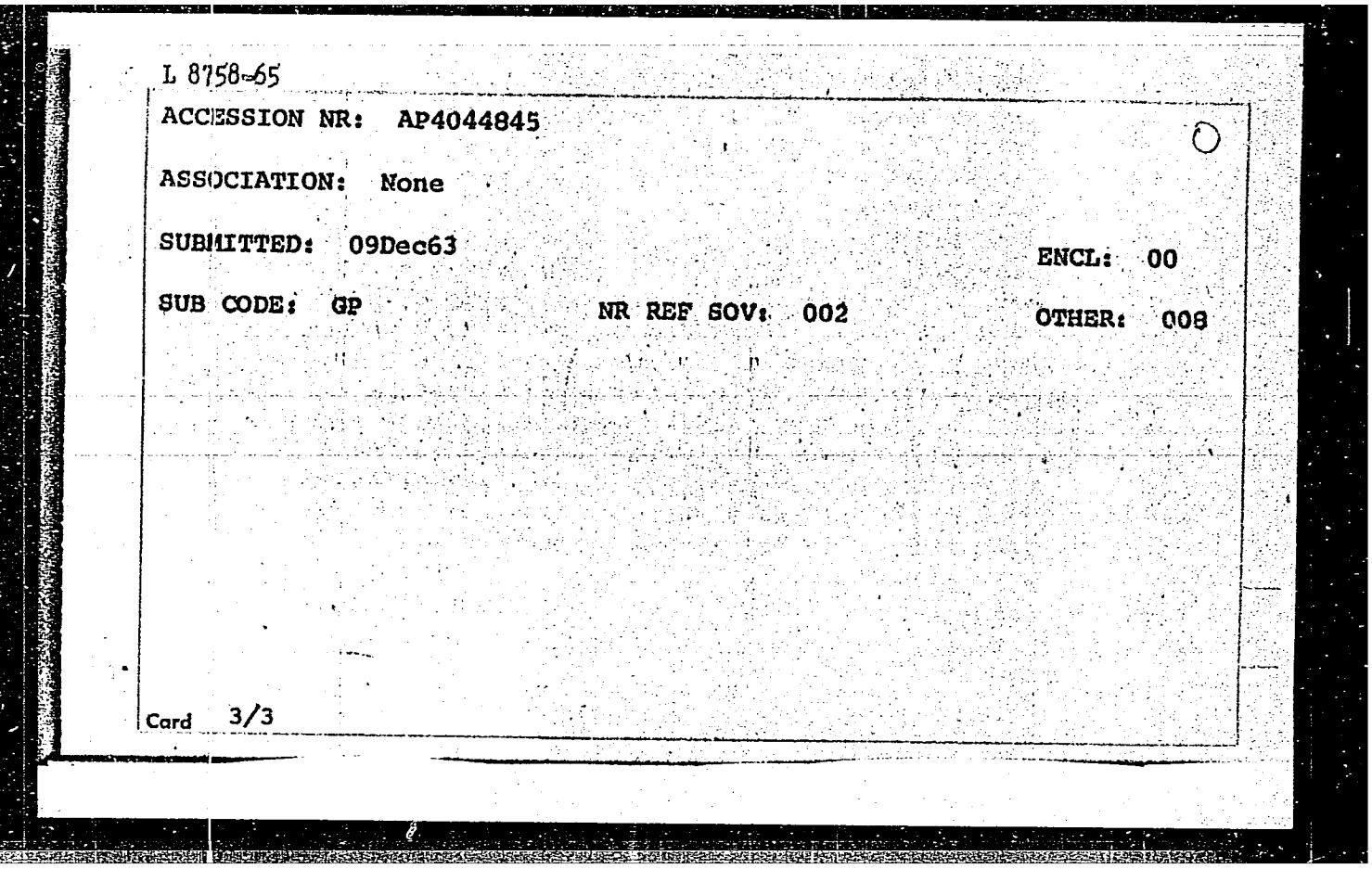


L 8758-65

ACCESSION NR: AP4044845

ASSOCIATION: None

SUBMITTED: 09Dec63 ENCL: 00

SUB CODE: GP NR REF SOV: 002 OTHER: 008

Card 3/3

SOKOLOV, N.D.

Relation between the frequency shifts of valence and deformation vibrations in the hydrogen bridge. Opt. i spektr. 17 no.3:455-456 S '64.
(MIRA 17:10)

SOKOLOV, N.D., doktor fiz.-matem.nauk

Conference on advances in Quantum Chemistry held at Kishinev. Vest. AN SSSR 34 no. 1:108-111 Ja '64. (MIRA 17:5)

ALEKSEYEV, Igor' Vladimirovich; LOKAYEV, N.I., otv. red.

[Theory of nuclear magnetic resonance] Teoriia iadernogo magnitnogo rezonansa. Moskva, Nauka, 1964. 206 p.
(MIRA 17:10)

PSHENICHNOV, Ye.A.; SOKOLOV, N.D.

Mechanism of reactions involving proton transfer in polar solvents. Kin. i kat. 6 no.5:802-808 S-O '65. (MIRA 18:11)

1. Institut khimicheskoy fiziki AN SSSR.

Sokolov, N.F.

21 621.3.014.31 : 621.316.3

2538. EXTINCTION OF A D.C. ARC IN A ROTATING MAGNETIC FIELD. A.E.Kapiyanskii, L.S.Polotovskii, N.F.Sokolov and P.I.Petrov.
Elektrichestvo, 1956, No. 12, 29-32. In Russian.

An experimental investigation showed that the extinction of the arc by a rotating magnetic field of commercial frequency is in many cases more efficient, in others not less efficient, than arc-quenching by means of a constant or pulsating field. The supply of arc-quenching devices with 3-phase current does not offer difficulties, since in practice the direct-current concerned will almost exclusively be rectified 3-phase current. In some cases the use of a rotating field will reduce the dimensions of the arc-quenching device, this rendering the method suitable for use in d.c. switchgear, electronic converters and contact rectifiers. The latter use was tried out on a model of a mechanical 3-phase rectifier the contacts of which were placed in a rotating magnetic field. Without application of the field strong sparking at the contacts occurred at currents of only 0.5 A and 30 V. With the field applied, visible sparking did not occur up to the limiting current loading of 150 A of the model. The flux density of the rotating field must be 360-500 Gauss.

B.F.Kraus

SOKOLOV, N.F.; PINSKER, A.L.

Problems in the improvement of technical means for producing new tractors and agricultural machines. Trakt. i sel'khozmash. no.12:28-34 D '58. (MIRA 11:12)

1. Nauchno-issledovatel'skiy institut Traktorosel'khozmash.
(Agricultural machinery industry)

SOKOLOV, N.F.

New automatic lines. Trakt.i sel'khozmash. 30 no.2:38-39 F '60. (MIRA 13:5)

1. Nauchno-issledovatel'skiy institut Traktorosel'khozmash.
(Agricultural machinery industry)

SOKOLOV, N.F.

Modernization of agricultural machinery plants. Trakt. i sel'khozmash. 31 no.7:34-37 Jl '61. (MIRA 14:6)

1. Nauchno-issledovatel'skiy institut tekhnologii traktornogo i sel'skokhozyaystvennogo mashinostroyeniya.
(Agricultural machinery industry)

LYSENKO, A.P.; SOKOLOV, N.F.; MIKHLIN, B.Z.

Methods of measuring weak magnetic fields in a wide spectrum of frequencies. Geofiz. prib. no.9:25-36 '61. (MIRA 15:11)
(Magnetism, Terrestrial--Measurement)

SOKOLOV, N.G., inzhener.

Universal square tubular transverse beam. Rats. i izobr. predl. v stroi. no.130:13 '56. (MLRA 9:9)
(Building blocks)

SOKOLOV, N.G., inzhener.

Device for filling vertical seams in large-block walls. Rats. i izobr. predl. v stroi. no.130:14 '56. (MLRA 9:9)
(Building blocks)

MAKSIMOVSKIY, N.P., kand.tekhn.nauk; SOKOLOV, N.G., inzh.

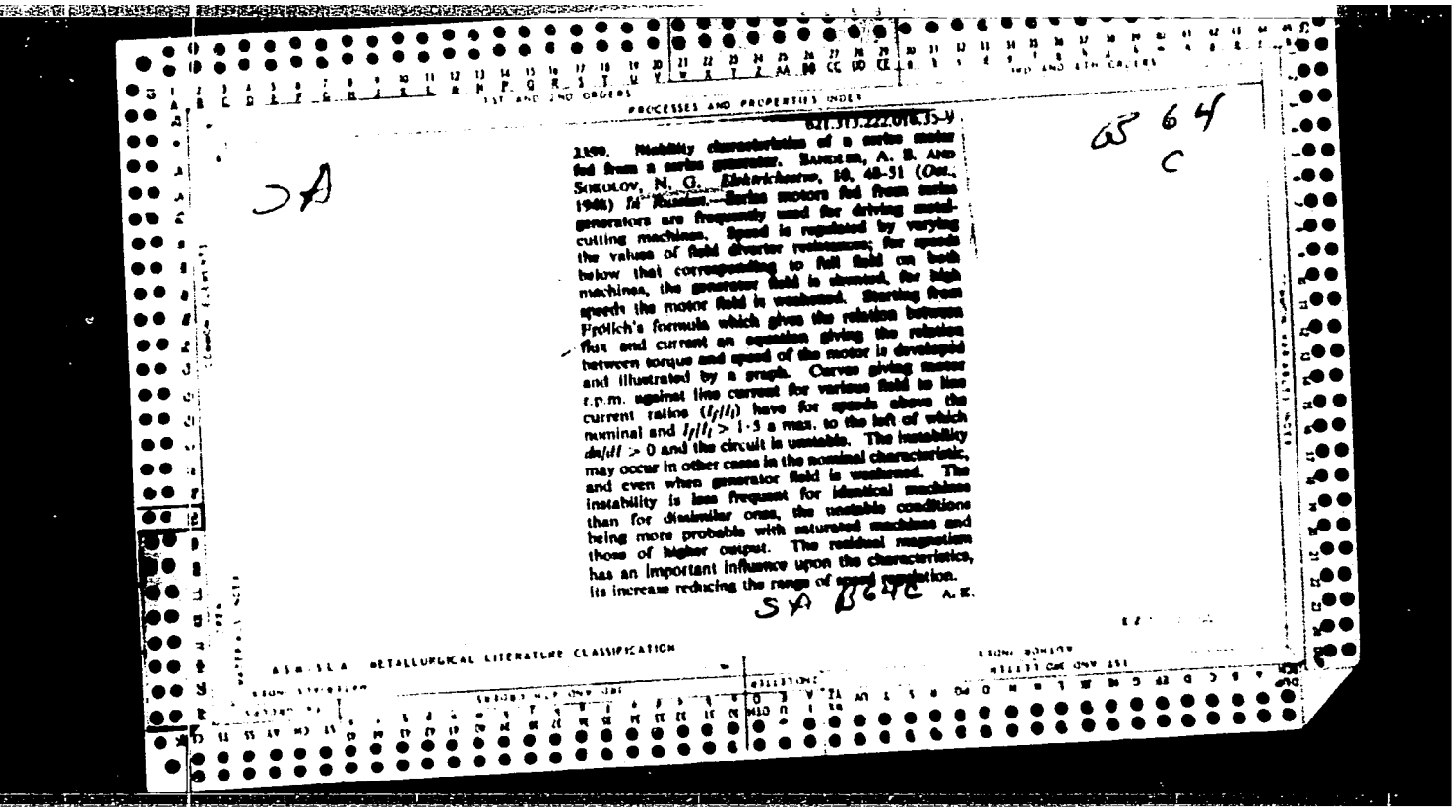
Making lightweight concretes for large panels and blocks using improved mixing machinery. Stroi. mat. 6 no.9:11-13 S '60. (MIRA 13:9)

(Mixing machinery) (Lightweight concrete)

SOKOLOV, M. G., Engr. Sci. Tech. Sci.

Dissertation: "Investigation of the Properties of a Series Motor Fed From a Series Transformer." Moscow Order of Lenin Power Engineering Inst imeni V. M. Molotov, 21 Nov 47.

SO: Vechernyaya Moskva, Nov, 1947 (Project #17836)



PROCESSES AND PROPERTIES INDEX

621.313.222.018.35-4

2199. Stability characteristics of a series motor fed from a series generator. Ramsim, A. B. and Sheglov, N. G. *Elektrichestvo*, 10, 48-51 (Oct., 1948) *In Russian.*—Series motors fed from series generators are frequently used for driving metal-cutting machines. Speed is regulated by varying the values of field diverter resistances; for speeds below that corresponding to full field on both machines, the generator field is shunted, for high speeds the motor field is weakened. Starting from Frolich's formula which gives the relation between flux and current an equation giving the relation between torque and speed of the motor is developed and illustrated by a graph. Curves giving motor r.p.m. against line current for various field to line current ratios (I_f/I_l) have for speeds above the nominal and $I_f/I_l > 1{\cdot}5$ a max. to the left of which $dn/dI > 0$ and the circuit is unstable. The instability may occur in other cases in the nominal characteristic, and even when generator field is weakened. The instability is less frequent for identical machines than for dissimilar ones, the unstable conditions being more probable with saturated machines and those of higher output. The residual magnetism has an important influence upon the characteristics, its increase reducing the range of speed regulation. A.E.

ASM-SLA METALLURGICAL LITERATURE CLASSIFICATION

8(5)

AUTHORS: Sirotin, Artemiy Afanas'yevich, Candidate of Technical Sciences, Docent at Kafedra elektrooborudovaniya prompredpriyatiy Moskovskogo energeticheskogo instituta (Chair of Electrical Equipment of Industrial Enterprises), Sokolov, Nikolay Georgiyevich, Candidate of Technical Sciences, Docent at the Chair of Electrical Equipment of Industrial Enterprises, Moscow Power Engineering Institute, Rubtsov, Vladimir Vasil'yevich, Engineer at the 1 Podshipnikovyy zavod g. Moskvy (1st Bearing Factory of the City of Moscow) SOV/161-58-2-24/30

TITLE: Electric Lag Drive of the Cross Feed (Transverse Feed) of Sphero-Grinders (Sledyashchiy elektroprivod poperechnoy podachi sferoshlifoval'nykh stankov)

PERIODICAL: Nauchnyye doklady vysshey shkoly. Elektromekhanika i avtomatika, 1958, Nr 2, pp 196 - 204 (USSR)

ABSTRACT: The system of the cross feed electric drive should secure the removal of the main part of the supply at the maximum admissible actual feed. The slight rest of the supply has to be removed from a feed which secures the necessary quality of the product surface at minimum time. These requirements are met by the lag drive of the cross-feed which was developed for sphero-

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grinders by the co-workers of the Moskovskiy energeticheskiy institut (Moscow Power Engineering Institute) in cooperation with the Pervyy gosudarstvennyy podshipnikovyy zavod 1GP3(First State Warehouse Factory 1GP3). The mode of effect of the lag system of cross feed is described and the electric wiring diagram of sphero-grinders with the lag drive of cross feed is shown. This system was fitted to the sphero-grinders of the Leningradskiy zavod imeni Il'icha (Leningrad Works imeni Il'ich) and to the machines of the Van-Norman works. The experimental investigation of the electric lag drive are described. The positive properties of the electric lag drive are as follows: 1) A check at the workshop has shown that this system meets the series production requirements of ball-bearing factories. 2) When correctly adjusted, the lag system prevents scrap of rings owing to burning. 3) The lag feed increases by efficiency a correct adjustment as compared to the existing mechanical facilities. 4) The surface quality at a lag feed is between the 7th and 8th class. 5) The lag feed permits an uncomplicated adjustment of one mode of operation to another. 6) The

grinder is protected against excessive wear. 7) The electric diagram is not more complicated. 8) The diagram is more reliable than in other cases, due to the use of semiconductor valves instead of thermionic valves. 9) It is an automatic feed. 10) The specific energy consumption is lower by 16.1% as compared to mechanical feed. 11)The kinematic diagram of the cross feed assembly is by far less complicated. There are 8 figures.

ASSOCIATION: Kafedra elektrooborudovaniya prompredpriyatiy Moskovskogo energeticheskogo instituta (Chair of Electrical Equipment of Industrial Enterprises, Moscow Power Engineering Institute)

SUBMITTED: February 10, 1958

SOKOLOV, Nikolay Georgiyevich; KLYUCHEV, V.I., kand. tekhn. nauk, retsenzent; KAPUNTSOV, Yu.D., inzh., retsenzent; ZIMIN, Ye.N., kand. tekhn. nauk, red.

[Design of electric drives for industrial mechanisms] Konstruirovanie elektroprivodov proizvodstvennykh mekhanizmov; posobie dlia studentov spetsial'nosti [Elektrifikatsiia promyshlennykh predpriiatii i ustanovok." Red.E.N.Zimin. Moskva, Mosk. energ.in-t, 1961. 222 p. (MIRA 16:6)
(Electric driving)